

Introduction to Machine Learning

KL for ML



Learning goals

- Understand why measuring distribution similarity is important in ML
- Understand the advantages of forward and reverse KL



MEASURING DISTRIBUTION SIMILARITY IN ML

- Information theory provides tools (e.g., divergence measures) to quantify the similarity between probability distributions

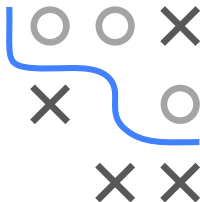
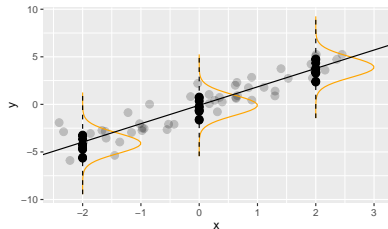


- The most prominent divergence measure is the KL divergence
- In ML, measuring (and maximizing) the similarity between probability distributions is a ubiquitous concept, which will be shown in the following.

MEASURING DISTRIBUTION SIMILARITY IN ML / 2

- **Probabilistic model fitting**

Assume our learner is probabilistic, i.e., we model $p(y|\mathbf{x})$ (for example, logistic regression, Gaussian process, ...).



We want to minimize the difference between $p(y|\mathbf{x})$ and the conditional data generating process $\mathbb{P}_{y|\mathbf{x}}$ based on the data stemming from $\mathbb{P}_{y,\mathbf{x}}$.

Many losses can be derived this way. (e.g., cross-entropy loss)

KL DIVERGENCE

Divergences can be used to measure the similarity of distributions.

For distributions p, q they are defined such that

- 1 $D(p, q) \geq 0$,
- 2 $D(p, q) = 0$ iff $p = q$.

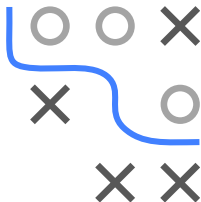
\Rightarrow divergences can be (and often are) non-symmetrical.

If the same measure dominates the distributions p, q , we can use KL.

For a target distribution p and parametrized distribution q_ϕ , we call

- $D_{KL}(p||q_\phi)$ forward KL,
- $D_{KL}(q_\phi||p)$ reverse KL.

In the following, we highlight some properties of the KL that make it attractive from an ML perspective.



KL DIVERGENCE / 2

- **Forward KL for probabilistic model fitting**

We have samples from the DGP $p(y, \mathbf{x})$ when we fit our ML model.

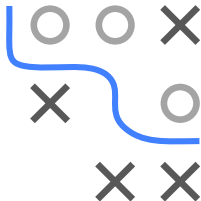
If we have a probabilistic ML model q_ϕ the expected forward KL

$$\mathbb{E}_{\mathbf{x} \sim p_{\mathbf{x}}} D_{KL}(p(\cdot|\mathbf{x})||q_{\phi}(\cdot|\mathbf{x})) = \mathbb{E}_{\mathbf{x} \sim p_{\mathbf{x}}} \mathbb{E}_{y \sim p_{y|\mathbf{x}}} \log \left(\frac{p(y|\mathbf{x})}{q_{\phi}(y|\mathbf{x})} \right).$$

We can directly minimize this objective since

$$\begin{aligned}\nabla_{\phi} \mathbb{E}_{\mathbf{x} \sim p_{\mathbf{x}}} D_{KL}(p(\cdot|\mathbf{x}) || q_{\phi}(\cdot|\mathbf{x})) &= \mathbb{E}_{\mathbf{x} \sim p_{\mathbf{x}}} \mathbb{E}_{y \sim p_{y|\mathbf{x}}} \nabla_{\phi} \log(p(y|\mathbf{x})) \\ &\quad - \mathbb{E}_{\mathbf{x} \sim p_{\mathbf{x}}} \mathbb{E}_{y \sim p_{y|\mathbf{x}}} \nabla_{\phi} \log(q_{\phi}(y|\mathbf{x})) \\ &= -\nabla_{\phi} \mathbb{E}_{\mathbf{x} \sim p_{\mathbf{x}}} \mathbb{E}_{y \sim p_{y|\mathbf{x}}} \log(q_{\phi}(y|\mathbf{x}))\end{aligned}$$

⇒ We can estimate the gradient of the expected forward KL without bias, although we can not evaluate $p(y|\mathbf{x})$ in general.



KL DIVERGENCE / 3

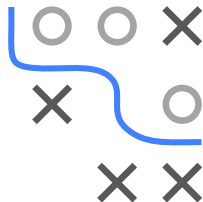
- **Reverse KL for VI**

Here, we know our target density $p(\theta|\mathbf{X}, \mathbf{y})$ only up to the normalization constant, and we do not have samples from it.

We can directly apply the reverse KL since for any $c \in \mathbb{R}_+$

$$\begin{aligned}\nabla_{\phi} D_{KL}(q_{\phi} \| p) &= \nabla_{\phi} \mathbb{E}_{\theta \sim q_{\phi}} \log \left(\frac{q_{\phi}(\theta)}{p(\theta)} \right) \\ &= \nabla_{\phi} \mathbb{E}_{\theta \sim q_{\phi}} \log \left(\frac{q_{\phi}(\theta)}{p(\theta)} \right) - \underbrace{\nabla_{\phi} \mathbb{E}_{\theta \sim q_{\phi}} \log c}_{=0} \\ &= \nabla_{\phi} \mathbb{E}_{\theta \sim q_{\phi}} \log \left(\frac{q_{\phi}(\theta)}{c \cdot p(\theta)} \right).\end{aligned}$$

\Rightarrow We can estimate the gradient of the reverse KL without bias (even if we only have an unnormalized target distribution)



KL DIVERGENCE / 4

The asymmetry of the KL has the following implications

- Forward KL $D_{KL}(p\|q_\phi) = \mathbb{E}_{\mathbf{x}\sim p} \log \left(\frac{p(\mathbf{x})}{q_\phi(\mathbf{x})} \right)$ is mass-covering since $p(\mathbf{x}) \log \left(\frac{p(\mathbf{x})}{q_\phi(\mathbf{x})} \right) \approx 0$ if $p(\mathbf{x}) \approx 0$ and $q_\phi(\mathbf{x}) \gg p(\mathbf{x})$.
- Reverse KL $D_{KL}(q_\phi\|p) = \mathbb{E}_{\mathbf{x}\sim q_\phi} \log \left(\frac{q_\phi(\mathbf{x})}{p(\mathbf{x})} \right)$ is mode-seeking (zero-avoiding) since $q_\phi(\mathbf{x}) \log \left(\frac{q_\phi(\mathbf{x})}{p(\mathbf{x})} \right) \gg 0$ if $p(\mathbf{x}) \approx 0$ and $q_\phi(\mathbf{x}) > 0$

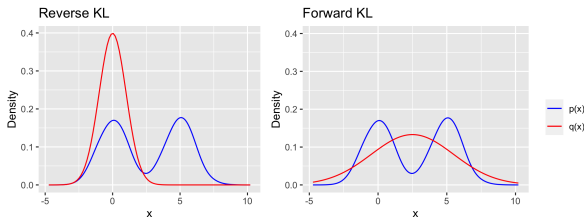


Figure: Optimal q_ϕ when q_ϕ is restricted to be Gaussian.